Workshop on Recent Developments in the Kondo Problem

January 9th - 10th 2015, ISSP, University of Tokyo

Title:

Workshop on Recent Developments in the Kondo Problem

Venue:

Institute for Solid State Physics, University of Tokyo

Date:

January 9th Fri. -10th Sat. 2015

Scope:

The last year 2014 is the 50-year anniversary of Prof. Kondo's paper "Resistance Minimum in Dilute magnetic Alloys" published in Prog. Theor. Phys. 32 (1964) 37, in 1964. Since then, the Kondo physics and the knowledge of the many-body theories developed around this topic have affected many fields in physics and continue to be actively researched. This workshop focuses on both theoretical and experimental developments in the Kondo physics in recent years:

- Quantum dot systems,
- Nonequilibrium properties,
- Heavy fermion systems,
- Numerical technique,

and any topic related to the Kondo physics.

The workshop will consist of both invited talks and contributed poster presentations giving a recent progress of research in the fields of the Kondo physics. We encourage participants in various fields to interact with each other and hope that this workshop will provide an opportunity for new collaborations.

Presentations:

Oral: 30mins presentation + 10mins question/discussion.
Poster: please put your poster before the poster session.

Organizer:

Rui Sakano, Yasuhiro Tada, and Kazumasa Hattori

Program

9 Jan. 2015 (Lecture Room A632)

13:05-13:10	Opening
13:10-13:50	Tomonori Shirakawa (RIKEN)
Fri 1	"Density-matrix renormalization group method for pseudogap Kondo problems"
13:50-14:30	Tetsuya Takimoto (Hanyang Univ.)
Fri 2	"Topological Kondo insulator"
14:30-15:10	Yosuke Matsumoto (ISSP, Univ. of Tokyo)
Fri 3	"Novel quantum criticality in valence fluctuating $YbAlB_4$ systems"
15:10-15:30	*coffee break*
15:30-16:10	Tatsuya Fujii (ISSP, Univ. of Tokyo)
Fri 4	"Nonequilibrium Kubo formula and shot noise in mesoscopic systems"
16:10-16:50	Meydi Ferrier (Univ. of Paris-Sud, and Osaka Univ.)
Fri 5	"SU(2) and SU(4) Kondo effect probed by nonequilibrium current fluctuations"
17:00-18:30	**Poster session**
19:00-21:00	*Banquet*

10 Jan. 2015 (Lecture Room A632)

9:30-10:10	Hiroaki Kusunose (Ehime Univ.)
Sat 1	"Anomalous Kondo effect due to orbital degeneracy"
10:10-10:50	Koichi Izawa (Tokyo Institute of Technology)
Sat 2	"Phase diagram in Pr1-2-20 system with non Kramers doublet ground state"
10:50-11:10	*coffee break*
11:10-11:50	Junya Otsuki (Tohoku Univ.)
Sat 3	"Dual fermion approach to the two-dimensional Kondo lattice"
11:50-12:30	Robert Peters (RIKEN)
Sat 4	"Explaining STM-measurements for impurities and heavy fermions via the Kondo proximity effect"
12:30-13:30	*lunch break*
13:30-14:10	Russell Deacon (RIKEN)
Sat 5	"Interplay between Kondo and proximity effect in hybrid superconductor-quantum dot devices"
14:10-14:50	~~Keiji Saito (Keio Univ.)~~ → Takeo Kato (ISSP, Univ. of Tokyo)
Sat 6	"Kondo signature in heat transfer via a local two-state system"
14:50-15:10	*coffee break*

15:10-15:50 Akira Oguri (Osaka City Univ.)

Sat 7 "Green's function for an SU(N) Anderson impurity: a comprehensive study with 1/(N-1) expansion, NRG, NCA, and exact high-temperature limit"

15:50-16:05 Concluding remarks, Kazuo Ueda (ISSP, Univ. of Tokyo)

Poster Presentation (17:00 – 18:30, 9 Jan.)

P01 Emi Minamitani (Univ. of Tokyo), "Underscreened Kondo state of collective spin in Mn-phthalocyanine on Pb(111)"

P02 Rui Yu (NIMS), "Novel surface spin textures for topological Kondo insulator SmB_6"

P03 Masaya Nakagawa (Kyoto Univ.), "Photo-induced Kondo effect in a two-orbital optical lattice"

P04 Takanori Taniguchi (ISSP), "NMR studies on quadrupole ordered phase in $PrTi_2Al_{20}$"

P05 Akihisa Koga (Tokyo Inst. of Tech.), "Valence fluctuations in the extended periodic Anderson model on the two-dimensional Penrose lattice"

P06 Tokuro Hata (Osaka Univ.), "Shot noise of a superconductor/nanotube junction in the Kondo regime"

P07 Koudai Iwahori (Kyoto Univ.), "Exact results for the periodically-driven impurity spin dynamics in a bath of ultracold fermions"

P08 Masaki Tsujimoto (ISSP), "Hybridization effects of quadrupolar moments in nonmagnetic compound PrV_2Al_{20}"

P09 Naoka Ohta (Univ. of Tokyo), "Two-dimensional molecular Kondo lattice"

P10 Ryoichi Hiraoka (Univ. of Tokyo), "Manipulating Kondo Hamiltonian in a molecular quantum dot"

P11 Kazuaki Takasan (Kyoto Univ.), "Photo-induced phase transition of topological Kondo insulators"

P12 Fuyuki Matsuda (Kyoto Univ.), "Analysis of valence transition in one-dimensional quasiperiodic Anderson-lattice model"

P13 Ryosuke Yoshii (Osaka Univ.), "Analytical study on interaction effect in quantum dot embedded in Aharonov-Bohm ring"

P14 Takahiro Tomita (ISSP), "Unconventional type of quantum criticality detached from the magnetic ordering in β-$YbAlB_4$"

P15 Kazuyuki Matsubayashi, (ISSP), "Pressure-temperature phase diagram of $PrTr_2Al_{20}$ (Tr = Ti, V) : interplay between quadrupole order and superconductivity"

P16 Yasuo Yoshida (ISSP), "Visualization of Ce atoms and site dependent in-gap residual density of state in $CeCoIn_5$"

Density-Matrix Renormalization Group Method for Pseudogap Kondo Problems

Tomonori Shirakawa[a,b], Robert Peters[a], and Seiji Yunoki[a,b,c]

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We have introduced a block Lanczos recursive technique to construct quasi-one-dimensional model, suitable for density-matrix renormalization group calculations, from single- as well as multiple-impurity Anderson models in any spatial dimensions [1]. The method allows us to calculate not only local but also spatially dependent static and dynamical quantities of the ground state for general Anderson impurity models without losing elaborate geometrical information of the lattice.

As a demonstration, we have applied the method to three different models for graphene with structural defect and with a single hydrogen or fluorine absorbed, where a single Anderson impurity is coupled to conduction electrons in the honeycomb lattice. These models include (i) a single adatom on the honeycomb lattice, (ii) a substitutional impurity in the honeycomb lattice, and (iii) an effective model for a single carbon vacancy in graphene. Our systematic analysis reveals that, for the particle-hole symmetric case at half-filling of electron density, the ground state of model (i) behaves as an isolated magnetic impurity with no Kondo screening, while the ground state of the other two models forms a spin-singlet state where the impurity moment is screened by the conduction electrons. We have also calculated the spin-spin correlation function between the impurity site and the conduction site. Our results clearly show that, the spin-spin correlation function decay as r^{-3} for model (i), and as r^{-4} for models (ii) and (iii) in the asymptotic r, where r is the distance between the impurity site and the conduction site.

We have also studied the entanglement spectrum of the ground state for the pseudo-gap Anderson impurity model. We have found that the lowest level of the entanglement spectrum is (a) four-fold degenerate in the Kondo screening phase, (b) two-fold degenerate in the local moment phase, and (c) non-degenerate in asymmetric strong coupling phase. We have found that the properties (a)-(c) are useful to determine the phase boundary.

Reference

[1] T. Shirakawa and S. Yunoki, Phys. Rev. B **90**, 195109 (2014).

Topological Kondo Insulator

Tetsuya Takimoto[a]

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In heavy electron systems, there is a class of insulators, whose resistivity increases exponentially below the temperature of resistivity minimum, i.e., Kondo insulators. The resistivity increases in the low temperature region due to opening a hybridization gap around the Fermi level. An actual example is a cubic compound SmB6. In SmB6, below the resistivity minimum around a room temperature, the common logarithm of resistivity increases by four down to 5 K, below which the resistivity is almost temperature independent[1]. In order to explain such a metallic behavior in the low temperature regime observed by various measurements, the so-called *in-gap* state has been introduced. The origin of in-gap state is still controversial.

After the prediction and the discovery of topological insulator, especially for Bi-compounds like Bi2Se3 and Bi2Te3[2-7], it has been proposed that some Kondo insulators can be classified into the topological insulator, based on a simple periodic Anderson model[8]. Recently, considering the realistic band structure of SmB6, we have calculated the topological index and the spectral function for surfaces of various direction[9]. As the result, SmB6 belongs to the class of strong topological insulator with ν_0=1, and the number of Dirac points in the surface spectral density is of odd independent of the direction of surface. Based on the result, the in-gap state is considered as the surface state of topological insulator.

Reference

[1] J.C. Cooley *et al.*,Phys. Rev. Lett. **74**, 1629 (1995).
[2] C.L. Kane and E.J. Mele, Phys. Rev. Lett. **95**, 146802 (2005).
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Novel quantum criticality in valence fluctuating $YbAlB_4$ systems

Yosuke Matsumoto, Takahiro Tomita, Kentaro Kuga, Eoin C. T. O'Farrell,
Yasuyuki Shimura and Satoru Nakatsuji

Institute for Solid State Physics, University of Tokyo, Japan.

Quantum criticality (QC) in heavy fermion systems has been studied mainly for Kondo lattice systems with integer valence where a quantum critical point is usually expected to be on the border of magnetism. On the other hand, the first Yb-based heavy fermion superconductor β-$YbAlB_4$ provides a unique example of QC in the mixed valent compounds [1, 2, 3, 4]. In addition, the QC cannot be explained by the standard spin fluctuation mechanism and emerges without tuning any control parameter, indicating formation of a strange metal phase [4]. Recent resistivity measurements under pressure have revealed that a non-Fermi liquid phase is stable over a finite pressure range up to ~ 0.4 GPa [5], which supports this idea. Here we review such novel phenomena observed in β-$YbAlB_4$ as well as those found in its isostructural polymorph α-$YbAlB_4$ discussing a possible role of valence fluctuation and anisotropic hybridization. In particular, we will discuss a sharp valence crossover induced by a chemical substitution in α-$YbAlB_4$ where we found a pronounced NFL behavior as a possible evidence of a quantum valence criticality [6]. These works have been done in collaboration with P. Coleman, A. H. Nevidomskyy, T. Sakakibara, Y. Uwatoko, Y. Karaki, K. Sone, J. Hong, S. Suzuki, H. Cao, D. MacLaughin, M. Okawa, Y. Takata, M. Matsunami, R. Eguchi, M. Taguchi, A Chainani, S. Shin, Y. Nishino, K. Tamasaku, M. Yabashi, T. Ishikawa, Y. Kiuchi, D. Hamane, M. Isobe, M. Koike. We thank them for their contributions.

Reference

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Nonequilibrium Kubo formula and shot noise in mesoscopic systems

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Advance of nanotechnology has allowed us to address the correlated transport in mesoscopic devices. Kondo effect in a quantum dot is one of fascinating examples. Recently shot noise in the Kondo regime has been studied. Especially in Refs.[1, 2], the Fermi-liquid nature has been reexamined. They have shown that the current close to the unitarity limit is given by $I = 2e^2V/h - I_b$ using "the backscattering current" I_b. It has thus stimulated to estimate an effective charge for the backscattering current. They have shown that the Fano factor $F_b = S/2eI_b$ results in a universal fractional value $5/3$ up to $\mathcal{O}(V^3)$. This universal feature has stimulated further studies. A shot-noise measurement has been reported on $F_b = 5/3$ close to the unitarity limit at low bias voltages[3]. In the context of the full counting statistics[4] this result has been reproduced and an expression in any strength of Coulomb interaction has been conjectured .

Here we prove the conjectured result in any strength of Coulomb interaction by using the renormalization perturbation theory(RPT). As shot noise, we use a new formula of shot noise S_h in the following discussion.

Recently we have deeply analyzed the density matrix of the Keldysh formalism applied for mesoscopic systems. The resulting density matrix enables us to obtain an expression of differential conductance: $G = \beta S/4 - \beta S_h/4$, where S is the current-current correlation function, and S_h is the non-trivial current-charge correlation function and $\beta = 1/k_{\mathrm{B}}T$[5, 6]. We have called it the *nonequilibrium Kubo formula*. The nonequilibrium Kubo formula is written into $S_h = S - 4k_{\mathrm{B}}TG$. At zero temperature S_h equals the conventional shot noise S. In the linear response regime S_h is proven to vanish, and the Nyquist-Johnson relation is reproduced. Furthermore in noninteracting systems $S^0 - 4k_{\mathrm{B}}TG^0$ expresses shot noise. Therefore we have proposed that S_h gives a definition of shot noise at any temperature in correlated systems. Thus theoretically calculated S_h can be compared with $S - 4k_{\mathrm{B}}TG$ using S and G measured in experiments. Therefore, the nonequilibrium Kubo formula enables us to address shot noise at any temperature in correlated systems[5].

Appling S_h to a quantum dot at zero temperature, the Fano factor $F_b = S_h/2eI_b$ is calculated using the RPT, and shown as

$$F_b = 1 + \frac{4(R-1)^2}{1+5(R-1)^2}, \tag{1}$$

where R is the Wilson ratio. Using limiting values of the Wilson ratio R, F_b yields

$$F_b = \begin{cases} \dfrac{5}{3} & U \to \infty \quad R = 2 \\ 1 & U \to 0 \quad R = 1 \end{cases} \tag{2}$$

F_b indeed reproduces the universal fractional value of $F_b = 5/3$ derived in the s-d limit, and a naively expected value $F_b = 1$ for a noninteracting system. Therefore eq.(1) indeed gives the general expression in any Coulomb interaction strength[6, 7].

References

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Fri 5

SU(2) and SU(4) Kondo effect probed by nonequilibrium current fluctuations

Meydi Ferrier[a,b], Tokuro Hata[a], , Tomonori Arakawa[a], Ryo Fujiwara[a], Raphaëlle Delagrange[b], Richard Deblock[b], Rui Sakano[c], Akira Oguri[d] and Kensuke Kobayashi[a]

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[d] *Department of Physics, Osaka City University, Japan*

Since 1980s mesoscopic conductors have been serving as ideal test-bed to investigate quantum scattering problems, because the quantum transport through a single site can be probed by electric measurements in a tunable way. Usually, researchers mainly investigate the current (or the conductance) that is the average number of electrons that pass through the system for a finite time. On the other hand, the fluctuation of the current ("shot noise"), namely the fluctuation of the number of electrons passing through it, conveys us very unique information. Combining transport and current noise measurements, we have unambiguously identified the SU(2) and SU(4) symmetries of quantum liquid in a carbon nanotube tuned in the Kondo regime [1]. We find that, while the electronic transport is well described by the free particle picture around equilibrium, the two particles scattering due to residual interaction emerges out of equilibrium. Most notably, we have extracted an effective charge for both symmetries in good agreement with theory [2].

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Anomalous Kondo effect due to orbital degeneracy

Hiroaki Kusunose[a]

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Orbital degrees of freedom in a magnetic ion increase variety to Kondo effect. I will show some examples showing anomalous Kondo effect, as a consequence of local competition between distinct ground states.

The highest symmetric generalization with orbital degeneracy is the SU(N) Coqblin-Schriffer model, which can be viewed as multipolar Kondo exchange model. Focusing on the time-reversal property of multipoles, we find that the model has an additional non-Fermi-liquid (NFL) fixed point in the presence of particle-hole (PH) symmetry without electric exchange coupling [1]. The spectral intensity of the quadrupole susceptibility diverges in the zero-frequency limit, while the dipole susceptibility shows a Fermi-liquid (FL) behavior. Such dual behaviors sustain themselves significantly for a fairly PH asymmetric case with the FL ground state.

The even number of f-electron valency in U and Pr (f^2 configuration) ions provides nonmagnetic crystalline-electric-field (CEF) states free from the Kramers theorem. Among them, a singlet CEF ground state can compete with the Kondo singlet. The puzzling behavior of $R_{1-x}U_xRu_2Si_2$ (R=Th, Y and La, $x \leq 0.07$) can be understood by such competition between two distinct FL fixed points [2]. Another interesting case is a non-Kramers CEF doublet ground state in cubic symmetry, which is a necessary condition for the two-channel Kondo model [3]. By considering a role of excited CEF states, there exists a competition between magnetic and quadrupole Kondo effects [4], in which the latter leads to NFL fixed point, while the former leads to FL fixed points. Relevance to the observed anomalous behaviors in PrT_2X_{20} (T=Ti, V, Ir, X=Al, Zn) will be discussed.

Reference

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[2] S. Yotsuhashi, K. Miyake, and H. Kusunose, J. Phys. Soc. Jpn. **71**, 389 (2002).
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Sat 2

Phase diagram in Pr1-2-20 system with non Kramers doublet ground state

Koichi Izawa[a], Taichi Yoshida[a], Toru Ikeura[a], Yo Machida[a], Takahiro Onimaru[b], Keisuke Matsumoto[b], Toshiro Takabatake[b], Akihito Sakai[c], Masaki Tsujimoto[c], and Satoru Nakatsuji[c]

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Rare-earth and actinide compounds with *f*-electrons display a variety of phenomena including magnetic order, multipole order, mixed valence, heavy-fermion, metamagnetic transition, non-fermi liquid behavior near a magnetic quantum critical point, unconventional superconductivity, etc. These phenomena reflect the quantum state of the electrons derived from the atomic *f*-orbitals via the hybridization between conduction and *f*-electrons. In fact, most of phenomena have been explained in terms of the interplay between Kondo effect and magnetic (RKKY) interactions, i.e. the Doniach picture, in which magnetic dipoles play an important role. On the other hand, the nature of electronic states characteristic of multipoles instead of magnetic dipoles remains unclear because of the lack of suitable systems.

Recent discovered praseodymium based 1-2-20 compounds PrT_2Zn_{20} (T=Ir, Rh) and PrT_2Al_{20} (T=Ti, V) provide a rare opportunity to study the nature of novel electronic states inherent in multipole degrees of freedom because they have a non-Kramers Γ_3 doublet ground state with only multipole degeneracy. In fact, *unusual* non-Fermi liquid behaviors reminiscent of the quadrupole Kondo effect were observed at low temperatures down to transition temperature of a long-range quadrupole order [1,2]. Moreover, superconductivity was found deep inside the ordered state, implying a role of quadrupole in the formation of Cooper pairs. However, the physics behind these phenomena is still far from being clarified. Here, based on our recent results of transport coefficients, we discuss the nature of novel electronic states and the phase diagram in non-Kramers doublet system in terms of quadrupole degrees of freedom.

Reference

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[2] A. Sakai *et al*., J. Phys. Soc. Jpn. **81**, 083702 (2012).

Dual fermion approach to the two-dimensional Kondo lattice

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Magnetism and superconductivity appear nearby in typical phase diagrams of strongly correlated electron systems, indicating correlation between them. Addressing such systems requires a unified treatment of magnetism and superconductivity. So far, unconventional superconductivities have been treated by variants of perturbation theory such as the fluctuation exchange approximation (FLEX). On the other hand, strong local correlations, which are responsible for formation of a local moment and hence for magnetism, can be described by the dynamical mean-field theory (DMFT). Therefore, it is highly desirable to construct a FLEX-like approximation on the top of the DMFT.

For this purpose, Rubtsov *et al.* introduced an auxiliary fermion (dual fermion) which “decouples” the kinetic-energy term of electrons [1]. This transformation enables us to perform a perturbation expansion around the DMFT; the zeroth order approximation in this theory corresponds to the DMFT, and spatial correlations are systematically incorporated by summing up a series of diagrams. In particular, ladder diagrams similar to those in the FLEX yield descriptions of long-range correlations [2]. Indeed, a phase diagram thus obtained for the two-dimensional Hubbard model exhibits d-wave superconductivity as well as the Mott insulating phase [3]. Therefore, the dual fermion approach gives a combined description of strong local correlations in the DMFT and long-range correlations in the FLEX.

We apply the dual-fermion approach to the two-dimensional Kondo lattice to investigate heavy-fermion superconductivities. Particular attention is given on the regimes near quantum critical points of two known instabilities: antiferromagnetism and charge-density wave. Which types of superconductivities are favored by those fluctuations will be discussed.

References

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Explaining STM-measurements for impurities and heavy fermion systems via the Kondo proximity effect

Robert Peters

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Recent progress in Scanning-Tunnel-Microscopy (STM), has made it possible to locally observe the Kondo resonance at the Fermi energy in the density of states (DOS) at very low temperatures. It has thereby been found that the Kondo-resonance in the DOS is not only visible directly at the impurity, but also at places away from it. Furthermore, it has been observed that the shape of the resonance depends on the place of the STM-measurement.

In this talk I will show that the Kondo-effect, induced by correlation effects on the impurity or within the f-electrons of the heavy fermion material, influences all other electrons in its vicinity, and is thereby observable also in the local DOS measured by STM at different atoms. I will theoretically analyze for two examples how the Kondo effect influences the DOS at different places: 1) In the first example, I will study the long-range Kondo effect of Fe- and Co-impurities buried below the Cu-surface [1]. The anisotropy of the Fermi surface of Cu leads to a strongly directional propagation of the Kondo effect, which is visible on the Cu-surface, even if the impurity is buried several layers below the surface. The shape of the resonance thereby changes, depending on the depth of the buried impurity. 2) The second example, which I will study, is related to recent STM experiments on heavy fermion systems such as CeCoIn5 [2]. The Kondo effect induced by the f-electrons of Ce is not only visible in the local DOS of Ce, but also in the local DOS of all other layers. Also in this system, it has been found that the shape of the resonance changes from layer to layer. In these heavy fermion systems, the Kondo resonance of the Ce-atoms propagates to the surrounding atoms and changes thereby its shape, which is observable in the STM experiment [3,4].

Reference

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Sat 5

Interplay between Kondo and proximity effect in hybrid superconductor-quantum dot devices

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The Kondo effect and superconductivity are two textbook many-body correlated states in condensed matter physics. The Kondo effect emerges in a quantum dot device when delocalized conduction electrons in the leads screen a localized spin on the dot resulting in a resonance level at the Fermi energy. The Kondo state is a spin singlet characterized by the Kondo temperature, T_K. The ground state of an 's'-wave superconductor is also a singlet characterized by the superconducting energy gap. When a quantum dot is contacted by superconducting leads the lack of low energy excitations inside the superconducting gap prevents the spin flip processes required for Kondo screening. As such superconductivity and Kondo effect act in competition. Despite this in devices with large T_K the Kondo effect and superconductivity can coexist. In this presentation the experimental work studying the competition between Kondo physics and superconductivity in quantum dot devices will be reviewed.

Sat 6

Kondo Signature in Heat Transfer via a Local Two-State System

Keiji Saito[a], and Takeo Kato[b]

[a] *Department of Physics, Keio University*
[b] *Institute for Solid State Physics, The University of Tokyo*

We study the Kondo effect in heat transport via a local two-state system. This system is described by the spin-boson Hamiltonian with Ohmic dissipation, which can be mapped onto the Kondo model with anisotropic exchange coupling. We calculate thermal conductance by the Monte Carlo method based on the exact formula. Thermal conductance has a scaling form with Kondo temperature T_k. Temperature dependence of conductance is classified by the Kondo temperature $(T/T_k)^3$ for very low temperature regime, while it has $(\frac{T}{\omega_c})^{2\alpha-1}$ for high temperature regime, where ω_c is a cut-off frequency and α is a dimensionless coupling strength. Similarities to the Kondo signature in electric transport are discussed.

Reference

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Green's function for an SU(N) Anderson impurity: a comprehensive study with $1/(N-1)$ expansion, NRG, NCA, and exact high-temperature limit

Akira Oguri,[a] Miyuki Awane,[a] and Rui Sakano[b]

[a] *Department of Physics, Osaka City University,*
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We study the Green's function of the N-orbital Anderson impurity in a wide range of the Coulomb interaction U, frequency ω, and temperature T, carrying out calculations using the $1/(N-1)$ expansion [1,2], the numerical renormalization group (NRG), the non-crossing approximation (NCA), and the exact asymptotic form that is available in the high-temperature limit and in the high-bias limit of a nonequilibrium steady state [3,4]. Comparisons of these approaches are made, specifically, for the $N = 4$ *particle-hole symmetric* case.

The $1/(N-1)$ expansion is a large N approach based on the perturbation theory in U, and uses a scaling that keeps $u = (N-1)U$ a constant in the limit of $N \to \infty$ [1,2]. At the zeroth order, it provides the Hartree-Fock (HF) approximation. Then, to leading order in $1/(N-1)$ it describes the Hartree-Fock random phase approximation (HF-RPA). Calculations are carried out up to order $1/(N-1)^2$ at which the fluctuations beyond the HF-RPA enter. The results show a reasonable agreement with the NRG results at low-energy Fermi-liquid regime. This approach is complementary to the NCA, which is based on the power series expansion in the hybridization matrix element V and keeps NV^2 finite for $N \to \infty$. We use the finite-U NCA to examine the T-dependence at intermediate temperatures.

The asymptotically exact high-temperature Green's function clarifies the detailed structure of N sub-peaks of the atomic nature, which appear at high frequencies as temperature increases. The result also correctly captures high-energy relaxation processes. It shows that the damping, or the level width of the sub-peaks, is determined by virtually excited $N-1$ particle-hole pairs in the Liouville-Fock space [3,4].

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P 01

Underscreened Kondo state of collective spin in Mn-phthalocyanine on Pb(111)

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The Kondo effect is one of the widely observed phenomena when contacting magnetic molecules to metal surfaces. In Mn phthalocyanine (MnPc) on Pb(111), the change of the Kondo temperature due to the quantum-well state formation [1] and the competition between Kondo effect and the superconductivity [2] in Pb substrate has been observed experimentally. However, the mechanism and detail of the Kondo state in MnPc/Pb(111) is still controversial [1-3].

In this study, by combining the low-temperature scanning tunneling spectroscopy (STS), density functional theory (DFT), and numerical renormalization group (NRG) calculation, we show that a unique collective S=1 spin state consisting of magnetic moments in ligand π orbital and Mn d-orbitals occurs in MnPc on Pb(111), which causes the spatially extended underscreened Kondo resonance.

The detailed STS observation clarified that the spectral feature of the Kondo resonance is almost the same between the Mn site and the pyrrole ring. The DFT calculation shows that the ligand π orbital antiferromagnetically couples to the magnetic moment in Mn atom. The charge transfer to the ligand π orbital from Pb substrate induces the reduction of the total spin from S=3/2 of gas phase to S=1. The NRG calculation results reveal that the Kondo effect screens the half of the collective S=1 spin rather than screening the individual magnetic moments separately, which causes the spatially extended underscreened Kondo resonance and allows the coexistence of the Kondo effect and antiferromagnetic interaction between localized spins.

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Novel surface spin textures for topological Kondo insulator SmB_6

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Topological Kondo insulators have been proposed as a new class of topological insulators in which non-trivial surface states reside in the bulk Kondo band gap at low temperature due to strong spin–orbit coupling. The hallmark signatures of these gapless surface states are the helical spin structure, which can be observed in ARPES experiment. Samarium hexaboride (SmB_6) has recently emerged as a prominent candidate for topological Kondo insulator with three Dirac-like surface states on its (111) surface. Starting from the k·p method in combination with first-principles calculations, we systematically derive simple but sufficient effective Hamiltonians that capture the low energy quasi-particle structures of SmB_6. Using these effective Hamiltonians we can obtain both the energy dispersion and the spin texture of the topological surface states [1]. We hope our model Hamiltonians can facilitate further experimental investigations of this material.

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Photo-induced Kondo effect in a two-orbital optical lattice

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Kondo effect is a ubiquitous phenomenon in condensed matter physics, and new platforms which realize the Kondo effect provide us a fresh insight into this long-studied phenomenon. In this presentation, we propose a novel route to realize the Kondo effect using *light-matter interactions*, motivated by recent progress in ultracold atomic physics using alkaline-earth species [1-4]. We consider a two-orbital system consisting of a Mott insulator and itinerant free fermions, and apply an external ac field which induces the optical transition between the orbitals. The ac field plays a role of hybridization, and thus dissolves the Mott insulator into the free fermionic "bath" degrees of freedom, which is nothing other than the emergence of the Kondo effect. We elucidate this dynamical realization of the Kondo effect and describe the resulting heavy-fermion state, using Keldysh field-theoretical formalism and slave-boson representation. Furthermore, we clarify that the photo-induced Kondo effect has a remarkable feature due to the form of the optical coupling, which results in a novel SU(N)-breaking Kondo effect and may induce a unique phase, which can be dubbed a "component-selective Kondo insulator".

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P 04

NMR studies on quadrupole ordered phase in $PrTi_2Al_{20}$

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The Kondo effect is known as a typical manifestation of many-body phenomena originating from interaction between the magnetic dipole moments of conduction electron and localized f-electron. Theoretically, a quadrupole Kondo effect derived from the electric quadrupole degree of freedom has been proposed [1]. However it has not been observed experimentally. It is important to study rare earth compounds, in which the ground state is non-magnetic and has quadrupole moment.

$PrTi_2Al_{20}$ has a cubic structure Fd-3m. In this material, crystal field ground states of Pr 4*f* electrons are non-magnetic doublets. From the specific heat measurements, an anomaly is observed about 2 K [2]. However no anomaly was observed in the magnetic measurements [2]. In addition, the ultrasonic measurements indicate the quadrupole phase transition at 2 K [3].

Here we report the results of ^{27}Al-NMR in a single crystal $PrTi_2Al_{20}$. The NMR measurements have been performed in the quadrupole ordered phase and para magnetic phase with an applied magnetic field of 6.615 T along the <100> or <111> directions. Al atoms occupy the three sites, 16c, 48f and 96g, crystallographically in $PrTi_2Al_{20}$. Especially we focus on the 96g-Al sites. The splits of spectra are observed near the phase transition temperature with an applied magnetic field along the <111> direction. Assuming that the phase is ferro-quadrupole order and order parameter is O_{20}, we can explain the splits. In this presentation, we will also report the temperature and magnetic field dependence of the Knight shift and nuclear magnetic relaxation rate.

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P 05

Valence fluctuations in the extended periodic Anderson model on the two-dimensional Penrose lattice

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Quasiperiodic systems have attracted much interest since the discovery of quasicrystals [1]. One of the interesting examples is the rare-earth compound Au-Al-Yb with the intermediate valence [2]. In the quasicrystal $Au_{51}Al_{34}Yb_{15}$, quantum critical behavior bas been observed, while the approximant $Au_{51}Al_{35}Yb_{14}$ with the periodic structure exhibits conventional heavy fermion behavior. These should suggest that the quasiperiodic structure and strong correlations in the rare-earth system should play an important role in understanding low temperature properties.

To discuss how the valence is affected by electron correlations on the quasiperiodic lattice, we consider the extended periodic Anderson model [3] on the two-dimensional Penrose lattice, as a simple example. To study low-temperature properties in the system, we combine the real-space dynamical mean-field method with the non-crossing approximation. We find that the Coulomb repulsion between localized and conduction electrons does not induce a valence transition [3], but the crossover between the Kondo and mixed valence states, which is contrast to the conventional system. In the mixed-valence region close to the crossover, a nontrivial valence distribution appears characteristic of the Penrose lattice. We then discuss local electron correlations in the Penrose lattice [4].

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P 06

Shot noise of a superconductor/nanotube junction in the Kondo regime

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We measured the conductance and the shot noise of a carbon nanotube contacted by Pd/Al superconducting electrodes, in both SU(2) and SU(4) Kondo regime. Varying the gate voltage, two different electronic transport regimes can be observed: if the contacts are symmetric, we observe a multiple Andreev reflections (MAR) regime, governed by the transmission coefficients provided by the Kondo effect [1]. On the other side, if the contacts are asymmetric, the less coupled contact will play the role of a tunnel probe [2]. The conductance the reflects the energy of the Andreev bound states formed in the quantum dot and thus depends strongly on the ratio Δ/T_{K} , which determines if the ground state of the system is a Kondo singlet or a doublet. We measured the shot noise in both situations.

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P 07

Exact results for the periodically-driven impurity spin dynamics in a bath of ultracold fermions

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The dynamics of a single impurity in a fermionic or bosonic bath is one of the fundamental problems in condensed matter physics, and plays an important role in the X-ray absorption problem, polarons, Kondo effect and so on. Recently, these impurity problems are studied in the ultracold atomic systems. For example, a polaronic system is experimentally realized [1], and the realization of Kondo effect is theoretically proposed [2]. Due to the high controllability, dynamics of impurity driven by the time-dependent external field is also studied [3, 4].

Motivated by these studies, we investigate the periodically-driven impurity spin dynamics coupled to an ultracold fermionic bath by Kondo coupling. In general, even in the noninteracting case, it is difficult to solve the dynamics of the periodically driven quantum system analytically. Thus we consider the case that the external field changes values discretely in time and the Hamiltonian is at the special point in the parameter space (Toulouse limit) at which we can solve each time-step analytically, and thereby treat the full dynamics exactly.

First, in arbitrarily-discretized field cases, we find that the expectation values of impurity spin and fermions' spin in the bath oscillate with a frequency depending on the intensity of the external field and follow the external field in the time scale of Kondo temperature. Then, we calculate these values in the cases of rectangular field and sinusoidal field discretized appropriately. As a result, we find that their behavior changes with the field-intensity h, the frequency Ω, and the Kondo temperature T_K. In $h \gg \Omega, T_K$, they oscillate with the frequency of $2\pi/h$, while in $\Omega \gg h, T_K$, they approach a temporally constant value.

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P 08

Hybridization effects of quadrupolar moments in nonmagnetic compound PrV_2Al_{20}

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Quantum criticality due to the magnetic hybridization between *f* electrons and conduction electrons has been studied intensively and is known to lead to various interesting phenomena such as strange metallic behavior and unconventional superconductivity. On the other hand, the existence of quadrupolar version of Kondo effect and the quantum critical point (QC) have not been established. Thus, it is interesting to realize the quadrupolar Kondo effect and the QCP in real materials.

One of the best candidates for the study of hybridization effects due to quadrupolar moment is $PrTr_2Al_{20}$ (Tr : Ti, V). The crystal structure is cubic, and the crystal electric field (CEF) ground state of Pr is the cubic non-magnetic Γ_3 doublet [1,2]. Both materials exhibit quadrupolar ordering under T_Q = 2.0 K (Ti), 0.6 K (V) [1]. Furthermore, the strong hybridization effects have been observed, such as the Kondo effect in resistivity and the Kondo resonance peak in photoemission spectroscopy [1,3]. PrV_2Al_{20} have smaller lattice constant than that of $PrTi_2Al_{20}$ and shows stronger hybridization effects. PrV_2Al_{20} shows anomalous metallic behavior in higher temperature region than T_Q, and moreover, that system shows heavy fermion superconductivity below T_c = 50 mK in the ambient pressure [4].

Thus, PrV_2Al_{20} is very appealing material for the study of quadrupolar Kondo effect which shows strong hybridization and has nonmagnetic ground state. In the presentation, various interesting behaviors derived from quadrupolar hybridization in PrV_2Al_{20} will be discussed.

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Two-dimensional molecular Kondo lattice

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Advance in scanning tunneling microscopy and spectroscopy (STM/STS) allows us to investigate Kondo effect of an isolated magnetic impurity at metal surface with high energy and spatial resolutions. Iron phthalocyanine (FePc) on Au(111) is an interesting model system for Kondo physics. The FePc molecule takes S=1 triplet spin state in the bulk. The two localized spins are coupled with the substrate electrons and are collectively screened so that Fano-Kondo (FK) resonances emerge in the STS spectrum [1]. In addition, one of the FK resonances evolves from single impurity regime to the two-dimensional lattice due to the competition of the Kondo screening with the magnetic interactions between the molecular spins: a single FK dip is split to a double-dip structure [2]. We investigated the spectral response of the square lattice of FePc on Au(111) to external magnetic fields by STM and STS. We found that the square lattice consists of two sublattices by spatial mapping of the spectral intensity under a magnetic field. This indicates the antiferromagnetic order develops in the molecular Kondo lattice [3]. We also found that the magnetic anisotropy is key to understand the spectral response to the magnetic field.

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Manipulating Kondo Hamiltonian in a molecular quantum dot

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Magnetic molecule on metal substrate has gathered lots of attention from both fundamental and applications viewpoints. Iron phthalocyanine (FePc) molecule takes S = 1 triplet spin state derived from the Fe^{2+} ion in the bulk and the spin-orbit coupling (SOC) lifts the degeneracy of S = 1. When adsorbed on Au(111), the two localized spins are coupled with the substrate electrons to give rise to Kondo effects so that Fano-Kondo (F-K) resonances emerge in the STS spectrum [1]. Thus, FePc on Au(111) provides unique opportunity to get deeper insights on the competition of Kondo effect and SOC. Here we demonstrate the reversible crossover from the Kondo regime to the SOC regime by tuning the molecule-substrate (MS) coupling with STM manipulation [2]. Approaching the STM tip to the molecule, the MS coupling is decreased so that the asymmetric FK resonance is evolved gradually to a symmetric spectral shape relevant of the inelastic spin excitation associated with the SOC. The excitation energy increases with the decrease of MS coupling. This crossover indicates that the depression of Kondo effects together with the development of level splitting derived from the SOC is caused by the STM manipulation.

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P 11

Photo-induced phase transition of topological Kondo insulators

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Controlling the nature of matter by laser light is an important topic in strongly correlated electron systems. We investigate the phase transitions of topological Kondo insulator induced by the high-frequency laser light. The topological Kondo insulator is a strongly correlated insulator that has a surface state protected by time-reversal symmetry (TRS) [1]. The laser light affects the topological properties of the material and causes out-of-equilibrium phase transitions.

First we study the non-interacting case. We calculate the effective Floquet Hamiltonian, which gives the information of this system in the high-frequency limit. Even in the non-interacting regime, this system shows various topological phases. Especially when the light is circularly polarized, TRS is broken. Its breaking induces a quantum Hall phase and a Weyl semi-metallic phase.

Next we consider the effect of interaction by a slave-boson approach. With this approach, we can calculate the renormalization effect self-consistently and determine the Kondo temperature. It enables us to discuss Kondo physics under the periodic external field. We show how the interaction effect changes the phase diagram of the non-interacting case. Finally we will address the perspective of future study.

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Analysis of Valence Transition in One-Dimensional Quasiperiodic Anderson-Lattice Model

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Recently, heavy fermion systems in quasicrystals have attracted much attention after quantum critical phenomena were found in the quasicrystals. In the quasicrystal $Yb_{15}Al_{34}Au_{51}$, quantum criticality of valence fluctuations emerges, which is shown to be quite robust against pressure, while this robustness is not seen in its approximant crystals [1]. The research reported that low-temperature properties of magnetic susceptibility χ, NMR/NQR relaxation rate $(T_1T)^{-1}$, specific-heat coefficient C/T, and resistivity ρ agree very well with the theory of quantum valence criticality. A theoretical research to explain this robustness of quantum criticality has been done by considering a single cluster of $Yb_{15}Al_{34}Au_{51}$ [2].

Can this robustness of quantum criticality be seen in random systems or is it specific to quasiperiodic systems? To answer these questions, we focus on the effects of quasiperiodicity on the quantum criticality of valence fluctuations. We consider the one-dimensional (1D) quasiperiodic Anderson-lattice model, which has quasiperiodically ordered impurities. The Hamiltonian can be written as follows,

$$\mathrm{H} = \sum_{j\sigma} \varepsilon_f f_{j\sigma}^\dagger f_{j\sigma} + \sum_{<i,i'>\sigma} t_{ii'} c_{i\sigma}^\dagger c_{i'\sigma} + \sum_{j\sigma} \left(V_f f_{j\sigma}^\dagger c_{j\sigma} + V_j^* c_{j\sigma}^\dagger f_{j\sigma} \right)$$
$$+ U_c \sum_i (n_{i\uparrow}^c - 1/2)(n_{i\downarrow}^c - 1/2) + U_f \sum_i (n_{i\uparrow}^f - 1/2)(n_{i\downarrow}^f - 1/2) + U_{fc} \sum_j n_j^f n_j^c$$

where $f_{j\sigma}^\dagger (f_{j\sigma})$ and $c_{j\sigma}^\dagger (c_{j\sigma})$ are creation (annihilation) operators of the f-orbital and conduction orbital respectively, and $n_{j\sigma}^{\mathrm{f}} = f_{j\sigma}^\dagger f_{j\sigma}$, $n_{j\sigma}^{\mathrm{c}} = c_{j\sigma}^\dagger c_{j\sigma}$. The sites with an f-orbital are ordered as “Fibonacci word”, which is known as a method to construct 1D quasiperiodic orderings. To treat the correlation effect precisely, we use the density matrix renormalization group (DMRG) method. We find that a valence transition occurs in different ε_f at each site. This is consistent with the previous research, which showed that the robustness of quantum criticality comes from overlap of the critical regimes at each site. Moreover, we discuss the properties which are specific to the 1D quasiperiodic Anderson-lattice model. Also, the comparison between periodic, quasiperiodic, and random-potential models will be shown.

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P 13

Analytical study on interaction effect in quantum dot embedded in Aharonov-Bohm ring

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The Kondo effect stems from the many-body entanglement of an impurity spin with conduction electrons. The effective Kondo coupling between those spins are renormalized to large values when the temperature is lowered below the Kondo temperature T_K. The Kondo effect still attracts theoretical and experimental attentions, since its experimental realization in gated semiconductor quantum dots. One interesting and highly nontrivial extension of the basic Kondo model involves an Aharonov-Bohm (AB) ring with a Kondo impurity in the lower arm and interference with an upper reference arm (ABK ring).

As shown in [1-4], Kondo scattering has both elastic and inelastic components which exhibit interesting variations with energy scale. Since inelastic scattering is generally known to destroy interference effects, a correspondingly rich dependence of the conductance of ABK ring on temperature and flux is expected. Recently, the finite temperature behaviour of the AB ring was also considered. Ref. [2] studied the role of inelastic scattering on the visibility of AB oscillations through a large open ring with an embedded quantum dot. Various assumptions were made in this work including the idealized notion of a large `open ring' which relates the conductance to the scattering cross section. In this study, we avoid these assumptions, calculating the full conductance including contributions from multiple traversals of the ring, using the Kubo formula [5].

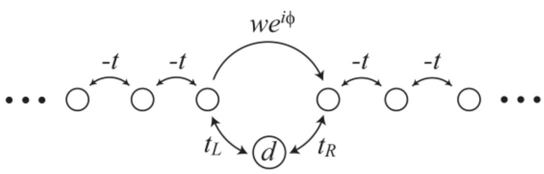

Fig: Quantum dot embedded in AB ring
Model of a quantum dot embedded in an Aharonov-Bohm ring. The leads are described by the tight binding model with hopping –t and upper arm is represented by direct tunneling.

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Unconventional type of quantum criticality detached from the magnetic ordering in β-$YbAlB_4$

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Recently discovered heavy fermion superconductor β-$YbAlB_4$ exhibits a field tuned quantum criticality despite strong mixed valiancy. [1,2] This material is also first discovered Yb-system showing the quantum criticality at zero temperature and zero field at ambient pressure. [3] This type of Yb electron system is expected that a *magnetic* order connected to the quantum critical point is driven through the application of *pressure*. So, we decided the pressure vs temperature phase diagram as a function of the Fe concentration by using the electrical resistivity, magnetization and specific heat measurements of single crystals β-$YbAl_{1-x}Fe_xB_4$ ($0 \leqq x \leqq 0.06$) down to the low temperature of 40 mK under pressure. [4] Here we observed that non-Fermi liquid $\rho \sim T^{1.5}$ showing at ambient pressure is robust with application of pressure up to 0.4 GPa. Additionally a crossover from non-Fermi-liquid $\rho \sim T^{1.5}$ to Fermi-liquid $\rho \sim T^2$ was observed. In further high pressure regime more than 2.5 GPa, the magnetic order was first observed and reaches at T_N = 30 K under 8 GPa. The same type of behavior is also confirmed in the Fe-doping as a function of chemical pressure. This is an unconventional type of quantum criticality detached from the magnetic ordering.

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Pressure-temperature phase diagram of $PrTr_2Al_{20}$ (Tr = Ti, V) : interplay between quadrupole order and superconductivity

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The Pr-based compounds with $4f^2$ configuration in the cubic crystal structure give an opportunity to investigate the role of the orbital degree of freedom, because the crystalline electric field (CEF) ground state of Pr ions can be a Γ_3 doublet state with an electric quadrupole moment. Since non-Kramers Γ_3 doublet ground state has no magnetic degrees of freedom, the electric quadruple moments cause exotic ground states such as the quadrupole ordering and the quadrupolar Kondo effect through the hybridization with a conduction electron [1-3]. More interestingly, recent work on Pr-based 1-2-20 compounds, $PrTr_2X_{20}$ (Tr = Ir, Rh, Ti, V and X = Zn, Al), which crystallizes in a cubic structure, has demonstrated the interplay of the quadrupole order and superconductivity [4,5]. In particular, $PrTi_2Al_{20}$ exhibits the pressure-evolution of the heavy fermion superconductivity as the system approaches the possible quantum critical point of the ferroquadrupole (FQ) order. In this presentation, we show the complete pressure-temperature phase diagram of FQ order and superconductivity in $PrTi_2Al_{20}$ up to 15 GPa across the QCP of the FQ order. We will also present the effect of pressure on antiferroquadrupolar system PrV_2Al_{20} with a stronger hybridization effect, and discuss the nature of novel electronic states in non-Kramers Γ_3 system on the basis of a generic phase diagram of quadrupole order hosting superconductivity.

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Visualization of Ce atoms and site dependent in-gap residual density of state in $CeCoIn_5$

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$CeCoIn_5$ is known as a heavy fermion compound naturally born at the quantum critical point with the highest superconducting transition temperature T_C=2.3 K among heavy fermion superconductors. Recently, several scanning tunneling microscopy and spectroscopy (STM/S) works on $CeCoIn_5$ successfully visualized the gradual formation of heavy quasiparticles with decreasing the temperature from 70 K to 20 K and nodal superconductivity with $d_{x^2-y^2}$ symmetry at low temperatures down to 245 mK [1-4]. However, there are some mysteries remained; missing Ce atoms in the Ce-In plane in the STM images and unusually large residual density of state (RDOS) within the superconducting gap even in the temperature range which is 10 times lower than T_C. Here we report the first observations of Ce atoms and large variation in the in-gap RDOS taken at the two different atomic sites, Ce and In, by precise STM/S measurements with extremely small tip-sample distances. The site-dependent in-gap RDOS is smeared out in fields and disappears above the critical field indicating that is intrinsic to the superconductivity. In the presentation, we discuss the results in the context of multigap superconductivity.

References:

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Important notice

◆The place has been changed from Seminar Room A615 to **Lecture Room A632** (大講義室: Dai-Kougi-Shitsu).

◆We do not provide WiFi access to you. In case of emergency, please visit registration desk.

< The Saturday, 10 Jan. >

Only the **South-West entrance** of the ISSP building is open from **9:00am to 16:00pm.**

In this early January, restaurant "Ikoi(憩い)", Cafeteria, and the Seikyo (food shop) are closed on Saturday. You can go to Sushi restaurant "Hama" in the campus (the number of seats is limited) or prepare your lunch box beforehand. There are several restaurants and convenience stores within 10min-walk distance from ISSP. We are very sorry for this inconvenience.

Map from Kashiwanoha-station to campus

◆banquet venue is restaurant *comesta* (1st floor in Mitsui Garden Hotel)